

# **Call for R&D Project Proposals on Exascale Systems: Application, Architecture and Software Under National Supercomputing Mission (NSM)**

Preamble:

The Department of Science and Technology (DST) in collaboration with the Ministry of Electronics and Information Technology (MeITy) has been implementing the National Supercomputing Mission project with the aim of ensuring country's leadership in supercomputing. As part of the initiative to ensure country's leadership in supercomputing, the country – the academia, R & D labs and the industry has already begun establishing a large repertoire of supercomputers with powers ranging from hundreds of Tera Flops to many Petaflops. These computers will be networked and would be available for the supercomputing community in India for research and development that will elevate the nation's science to be the best in the world. In order to harness this vast computing resource, to develop applications to tackle a broad spectrum nationally relevant and internationally competitive problems of unprecedented complexity working at peta and exascale and also to take the nation to the exascale era, it has been decided to initiate R & D projects across the country. This is the call for proposal on Exascale Systems: Application, Architecture and Software.

The focus would be on but not limited:

1. to build capabilities to tackle problems that are currently out of reach either for want of newer physics or newer algorithms
2. to focus on the use of machine learning and large scale data analytics at exascale level
3. to develop new programming models that scale well at exascale architectures
4. to develop popular application packages at peta and exscale level
5. to build newer class of processor architecture and interconnects.

The R&D activities/project proposals that are sought through this call would be broadly in the areas of

1. HPC Applications
2. Scalable Algorithms and Libraries
3. HPC System Software and Data Management
4. Hardware System Architecture
5. Enabling Technologies
6. Data Centre Infrastructure
7. Cross-cutting issues spanning across the above.

Key topics of interest in each of these areas include are, but not limited to, the following :

## **1. HPC Applications**

Computational problems in the following domains are of interest.

- Computational Physics, Astrophysics, Cosmology, Geophysics, High Energy Physics
- Computational Chemistry and Materials
- Material Genomics and material design
- Hybrid Classical-Quantum algorithms for scientific simulations
- Advanced/accelerated sampling methods, rare events methods
- Coarse-grained and multiscale modeling
- Computational Fluid Dynamics
- Weather Modeling and Climate Science

- Space
- Computational Biology
- Biomolecular, biomedical modeling, epidemiological modeling and simulation
- Omics (Genomics and other)
- Computational Neuroscience
- Drug Discovery
- Health
- Energy
- Combustion
- Fusion Energy and Nuclear Security
- Quantum models, algorithms and information sciences
- Cryptography and Cryptanalysis
- Information Security
- Network Science
- Smart Cities

In each of these areas, proposals aimed at the development of new computational methodologies, algorithms and applications addressing important problem areas are sought, especially scalable applications on exascale systems, as well as projects that aim to solve major scientific and engineering problems using computational approaches.

## **2. System Software**

In area of HPC System Software, the following problems are identified as important research topics:

- Programming models, Languages, Compilers and Runtime Systems for heterogeneous HPC systems
- Productivity, performance and power-aware Framework for HPC Applications
- Application/Workload characterization of Exascale Applications and their Power/Performance Estimation Methodologies
- Performance and scalability characterization, and scalability bottleneck identification tools for large-scale applications
- Middleware for HPC (Runtime environments, Communication, Scheduling, Fault tolerance and Reliability, Power-awareness, Job schedulers)
- Frameworks for multi-component HPC applications
- Data management Software for Big Data Scientific applications
- Data management across the deep-storage hierarchy in HPC
- In-situ data management
- Storage and Parallel File System, and I/O middleware systems for Exascale Systems
- Software systems for the efficient use of the deep-memory and non-volatile memory (NVM) hierarchy; solutions of storage class persistent memory and other emerging memory technologies
- OpenHPC System software and Tool Development for Exascale Platforms
- Code generators, auto-tuners and optimizing compilers
- Tools for performance tuning, correctness testing and debugging
- Workflow management systems for efficient end-to-end computing and distributed workflows

## **3. System Architecture**

The following problems are identified as important research challenges:

- Application Specific Acceleration Designs (Customized hardware) / Low Power Design and Reconfigurable hardware for HPC
- Low-power processor /accelerator design
- Interconnect network – Performance and Power-Aware designs, NoC designs
- Energy efficient HPC system design using low-power processors/memory, hybrid memory, compute-in-memory, etc.
- Heterogeneous system architecture designs
- Efficient Design Space Exploration
- Efficient hardware cooling designs/methods
- System architecture for data science and AI

#### **4. Scalable Algorithms & Libraries**

In the areas of Scalable Algorithm & Libraries, the research problems of interest include:

- Developing architecture- optimized mathematical libraries for heterogeneous architectures
- Auto-selection and auto-tuning of libraries
- Libraries for specific application domains
- Libraries for parallel I/O.
- Data analysis and visualization: Libraries and in-situ methods
- High-performance machine learning algorithms (HPC for ML) and Machine learning enabled HPC algorithms/simulations (ML for HPC)

#### **5. Enabling Technologies**

Under enabling technologies, newer technologies that will take HPC system design beyond Moore's Law will be explored. These include quantum, biological and quantum computing, quantum information sciences, neuromorphic computing, silicon photonics for high performance interconnect, approximate computing and in/near-memory computing, integration of compute, storage and network, etc.

#### **6. Data Centre Infrastructure**

Innovations in data center installation and integration, including research in power optimization, data center cooling, models and tools for heat flow in data centres and smart management, optimal rack design and cabling, are also encouraged.

#### **7. Cross-cutting Techniques**

Projects which cross-cut one or more of the above issues will also be of interest.

## **Guidelines**

### **Eligibility:**

All institutions who are eligible for DST/SERB Funding can apply.

### **Mode of Application and Selection:**

The call for applications will be notified through the websites of DST, MeITY, CDAC, IISc and JNCASR. Other host Institutions will also be requested to notify. The proposal in pdf format must be sent to [proposals.nsm@iisc.ac.in](mailto:proposals.nsm@iisc.ac.in). The selection will be based on the recommendations of an Expert committee.